

## LA-UR-21-23844

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Title: Associating damage nucleation and distribution with grain boundary characteristics in Ta

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Intended for: Web

Issued: 2021-04-20

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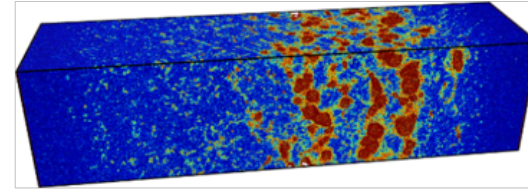
# Associating damage nucleation and distribution with grain boundary characteristics in Ta

Jie Chen and Saryu Fensin

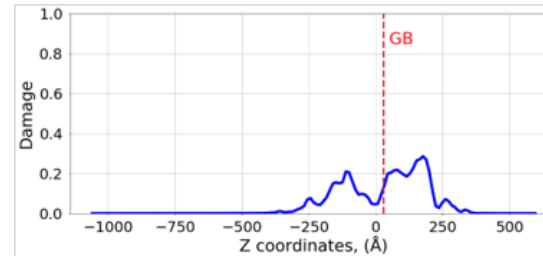
**Goal:** Develop a void nucleation criterion along with growth information as a function of material microstructure to provide input to damage models.

- Systematic molecular dynamics (MD) simulations were performed on 185 GBs in Ta.
- These GBs encompass both ordered and disordered structures – typically referred to as metastable structures, in order to reflect the diversity in the local atomic structure observed in realistic GBs.
- The results reveal four distinct regimes in damage distribution and failure modes as a function of misorientation angle, whereas variation in the local atomic structure does not affect the failure mode.
- The above trends also correlate with the variation in the corresponding void nucleation stress.

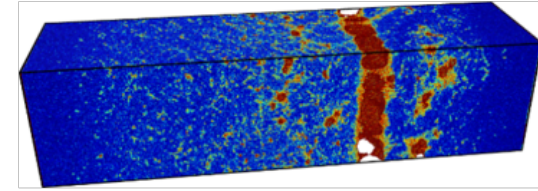
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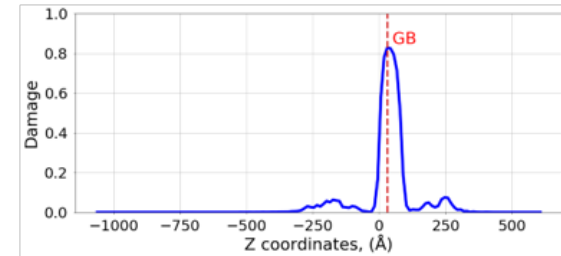
(a)



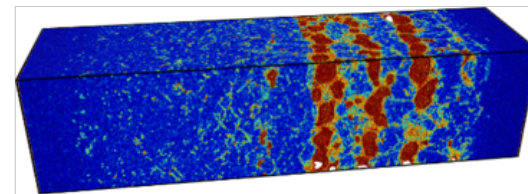
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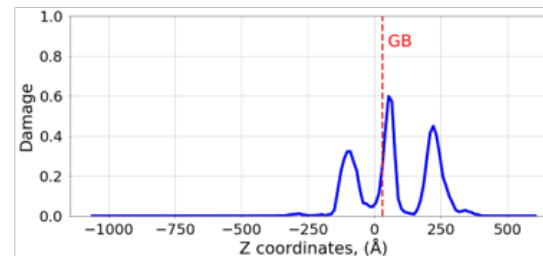
(b)



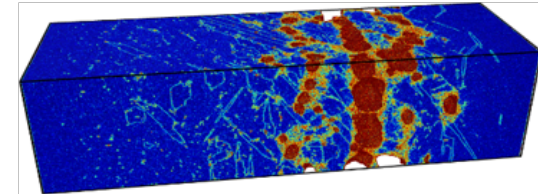
Regime 3



(c)



Regime 4



(d)

